

CCS News Bytes

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September-October 2005

CCS-5 Team's Expertise Helps Hurricane Victims

The simulation tools and expertise in the Discrete Simulation Science Group (CCS-5) are playing an important role this year in helping people who are trying to deal with a series of violent hurricanes.

Hurricane Studies

In an interview on September 22—two days before Hurricane Rita struck the Texas-Louisiana coast—Stephan J. Eidenbenz said that CCS had been asked four or five days before the projected landfall of Rita to provide estimates of how telecommunication systems would be affected by the storm. Because CCS-5 had done earlier studies on Houston infrastructure, the group had in hand data that made it possible “basically to do a full-fledged simulation,” he said.

Earlier, CCS-5 had been asked to prepare a post-event study on Hurricane Katrina, providing an estimate of the impact of that storm on telecommunication infrastructure in the New Orleans area.

“We looked at the networks that existed,” Eidenbenz said. “Then we tried to figure out which network elements were damaged—based on damage estimates and power outage estimates available shortly after the storm.”

“Most infrastructure elements fail,” he said, “because there is no power. They typically have battery backup power for a few hours. The larger switches have diesel generators. But these fail or run out of fuel after a couple of days.”

He added that the Decision Applications Division (D Division) provided a power outage map that was a key tool in helping CCS-5 determine the damage.

CCS-5 was able to propose a restoration order for switches damaged by Katrina. “To come up with this,” Eidenbenz said, “we ranked telecommunication elements relative to their importance. Because of the time pressure, we were not able to do a full-scale run of our simulation, but based on the expertise we have been building up from more detailed studies, we were able to make a good estimate.”

He said members of the CCS-5 team made a few calls to get single-point samples used to validate their estimates—but they kept the number of calls to approximately 20. “We were careful NOT to overload the network,” he said.

Asked if CCS-5 worked long hours to provide the necessary information, Eidenbenz said, “We did put in quite a few night shifts.”

“It was exciting,” he said. “It’s great to do work that has the potential to directly impact people’s lives in a good way.” Much of the group’s work is more long-term, he said. And he added that the work done on the two storms is likely to result in publications on the methods used.

CCS-5 knows that some of its reports were included in briefings at the Cabinet-Secretary level. Some were even sent on to the President.

“The team really worked great,” Eidenbenz said. He listed six people in addition to himself who were directly involved in the Katrina and Rita telecommunications response—Charles David Tallman, Sunil Thulasidasan, Matthew Nassr, CCS-5 Acting Group Leader James Smith (who provided coordination), Feng Pan of D Division, and Phil Romero of the Computing Communications and Networking Division.

(Please see CCS-5 on Page 4.)

Christon, Livescu Analyze Symposium's Success

What makes for a successful symposium?

The “Symposium on Modeling and Simulation of Variable Density and Compressible Turbulent Mixing,” held August 3-5 at Los Alamos National Laboratory (LANL), is viewed by many people as an outstanding success.

The reasons became clear in a recent interview with the organizers of the conference, Daniel Livescu and Mark Christon, both staff members in Continuum Dynamics (CCS-2).

(Livescu holds a Ph.D. in mechanical engineering from State University of New York in Buffalo. His specialty is fluid dynamics.

(Please see SYMPOSIUM on Page 2.)

SYMPOSIUM (Cont'd from p.1.)

(Christon has a doctorate in mechanical engineering from Colorado State University, specializes in computational fluid/hydro dynamics, and has been a staff member at both Lawrence Livermore National Laboratory and Sandia National Laboratories.)

Outstanding Speakers Draw Large and Varied Attendance.

The symposium—intended to foster a dialogue between researchers working on fundamental turbulence issues, numerical simulation, and modeling of variable density and compressible turbulent mixing—drew experts from LANL, Lawrence Livermore National Laboratory, and Sandia National Laboratories (both the Albuquerque and Livermore, California, branches). It also attracted outstanding people from academia and industry.

There were 20 unclassified invited talks.

The first day included, for example, talks by Norman J. Zabusky of Rutgers University (on “Vorticity Deposition and Evolution in Shock Accelerated Flows: Analysis, Computation, and Experiment”), Wai Sun Don of Brown University (on “Spectral Methods for Compressible Flows”); Paul Woodward of the University of Minnesota (on “Development and Validation of a Subgrid-Scale Compressible Turbulence Model”); Bhimsen Shivamoggi of the University of Central Florida (on “Theoretical Formulations for Intermittency in Compressible Fully Developed Turbulence”), and James Glimm, a member of the National Academy of Sciences who teaches at Stony Brook University (on “Modeling and Simulation of Turbulent Mixing in Real [Nonideal] Fluids”).

One of the speakers on the second day was Dale Pullin of California Institute of Technology, who spoke on “Large-Eddy Simulation of Richtmyer-Meshkov Instability.” Another was Alan Kerstein, a Senior Scientist at Sandia and a Fellow of the American Physical Society, who spoke on “A Strategy for High-Fidelity Computational Modeling of Flow, Mixing, and Reaction in Compressible Turbulence.”

The third day also featured excellent talks—all classified. Christon especially noted the high quality of the talks by two LANL staff members, Michael Bernardin and Miles Baron, both from LANL’s Applied Physics Division (X Division). He also mentioned presentations by Rebecca Darlington and Donald Roberts from Livermore.

More than 70 people attended the symposium. Livescu felt that people came “because the

speakers were among the best known in this field.” Christon said he was amazed that virtually everyone who registered for the conference actually attended. Livescu noted that people came not just because they were presenting, but also to listen to the talks of others. Christon commented that all three of the defense-oriented national laboratories were well represented. There was an especially good turnout from CCS, X, and the Theoretical Division (T Division) at LANL.

Early Preparation Defines Goals and Assures that They Are Met.

Preparations for the August symposium began in March.

Livescu, who chaired the first morning of discussions at the conference, said, “The idea didn’t come overnight.”

Christon, who served as chairman of the afternoon session on the first day of the symposium, recalled, “I was hoping to get back to doing more with large-eddy simulation, work that I had done in the past.” He knew Livescu because they were in overlapping fields, he said, “but that was about it.”

Livescu said, “We tried to make better connections with the top scientists in this field in the world” to improve the research activities in the field at LANL. A symposium, he said, is “a very good place to get new ideas and to expose your ideas to your peers.”

Christon recalled that, “People like Mark Chadwick (program manager in the nuclear weapons program directorate at LANL) wanted to inject some of these newer ideas into the ASC (the Advanced Simulation and Computing Program).”

Livescu said he and Christon talked with their group leader, John Turner, and with CCS colleagues Darryl Holm and Beth Wingate, and found that they all agreed that a symposium would improve work at LANL and make for better connections to the outside world. Finally, “It seemed a natural thing to do.”

Interactive Planning Draws on Wide Expertise.

“There are many conferences in this field,” Livescu said. “We wanted something that would not overlap with other conferences in the field and would benefit us most.”

(See MORE SYMPOSIUM on p.3.)

MORE SYMPOSIUM (From p.2.)

Christon said the preparation was interactive. "We surveyed a lot of people," he said, talking not only with people in CCS, but also with scientists in T Division and in X Division.

Livescu said it became apparent that there were two directions to follow at the symposium. The CCS organizers needed to connect with both the applied research in X Division and with the more theoretical approach in T Division.

Christon recalled that Chadwick, and Chuck Cranfill and Chong Chang of X-7, were especially helpful.

The final agenda had three types of talks. The first day presented computational talks; the second day featured modeling presentations; and the third day was devoted to applications.

Each session was followed by an unusual feature, a "second chance" session, during which speakers had an opportunity to clarify or expand on important points from their talks. Each day also featured roundtable discussion.

The symposium also made good use of LANL's own outstanding staff.

Malcolm Andrews (of CCS-2, P-23, and Texas A&M) served as chairman of the afternoon session on August 4.

The conference also tapped four scientists from Los Alamos as speakers. Andrews spoke on "Opportunities for Direct Numerical Simulation of Rayleigh-Taylor Mix Experiments." J.R. Ristorcelli (of X-7) spoke on "Initial Condition Dependence of Raleigh-Taylor Turbulence." Fernando Grinstein (also of X-7) spoke "On Implicit LES for Turbulent Flows." And Holm (of CCS-2 and Imperial College in London) spoke on "Introduction to LANS-Alpha, the Lagrangian Averaged Navier-Stokes Alpha Model of Turbulence."

In the abstract of a subsequent paper based on the conference, Christon, Livescu and Turner said:

"...The diverse cross-section of speakers permitted a broad sampling of advanced numerical methods, physical insight related to the applications of interest, and modern modeling approaches as the basis for answering the question 'How can advanced turbulence modeling approaches be used/extended for lab-centric applications?' The symposium provided a unique opportunity to survey state-of-the art approaches to turbulence modeling that ranged from moment closures to Large Eddy Simulations based on explicit stochastic and deterministic physical subgrid models, implicit

LES, the compressible Lagrangian averaging Navier-Stokes equations, variational multiscale and hybrid approaches. The issues associated with multi-fluid simulations, e.g., the importance of interface physics, were also addressed."

Useful Innovations Assist Future Efforts.

Livescu and Christon said they hope to hold another conference in the future. Livescu said it could take the form of a workshop at which "we could have some test problems or an important question to be answered, and people could work on these problems," or it could, once again, be a symposium on new material with formal talks and a roundtable.

They asked symposium participants to provide feedback to assess strengths and weaknesses and bring in good ideas for future meetings.

Livescu said the feedback is still coming in, but so far, the response has been excellent. He said one feature of the symposium that the participants especially liked was the "second chance" sessions.

A few examples illustrate the emerging trend in the feedback comments.

Pullin said, "I thought that the symposium was very successful. The discussions and comments at the end of each session were very good and were well organized."

Kerstein said, "My main impression of the symposium is that it provided a useful overview of the most important current approaches to turbulence and turbulent mixing simulation, presented by the leading developers and practitioners of the various approaches. Thanks again for the effort put into the organization of this very worthwhile event."

And Don said, "The organizers have done a great job in running the symposium. The presentation, speakers, and discussion were excellent."

Another decision that worked well, Livescu and Christon agreed, was having Tina Macaluso of Science Applications International Corporation (SAIC)-Advanced Systems Group take careful notes during the symposium. Livescu said CCS-2 had hired her to take notes at another CCS-2 meeting about a year earlier and liked the results. Her work at this conference made it much easier to prepare a meaningful summary paper afterward, they said.

(See TECHNICAL DETAILS, p. 4.)

TECHNICAL DETAILS (From p.3.)

For full scientific details of the conference, readers may view the paper, “LA-UR-05-7263, “Symposium on Modeling and Simulation of Variable Density and Compressible Turbulent Mixing Summary Report,” available on the CCS-2 website, <http://www.ccs.lanl.gov/ccs2/index.shtml>, or access the symposium website, located at http://www.ccs.lanl.gov/ccs2/msvdtm_symposium/

Afterward....

It is not unusual for symposium organizers to be tense as they work toward a successful outcome, but Livescu had a special reason for nervousness August 3-5: His first child was due any moment. Christon said that actually, his colleague was remarkably calm. The baby boy cooperated, waiting until the symposium was over to make his appearance on August 14.

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CCS-5 (Cont'd from p.1.)

Earlier Accomplishments

CCS-5 work was already drawing national attention even before Katrina hit. Scientists in the group did work involving both Hurricane Dennis in July and Hurricane Ophelia, the storm that went up the Eastern Seaboard in the days shortly after Katrina battered the Gulf Coast.

In a separate interview September 22, Smith listed a number of recent accomplishments. “The National Infrastructure Simulation and Analysis Center (NISAC) Urban Infrastructure Suite Project has made some amazing progress and had a tremendous impact over the past few weeks,” he said.

He pointed out that the project—using a combined team from CCS-5 and D Division to support Department of Homeland Security (DHS) deliverables—recently completed a major improvement in its entire simulation toolset *and* an analysis of the Los Angeles metropolitan area.

“Previous studies considered only a single, carefully scripted scenario in order to demonstrate the utility of these tools for DHS,” he said. “This was the first time a contingency analysis had been used for asset-loss consequence ranking to explore the broad range of possibilities in *all* sectors, and the first time the team produced a product to contribute to the National Asset Database.” He explained, “The results were used to rank order the criticality of the infrastructure assets so that DHS can plan its protection efforts.”

To put this accomplishment into perspective: Los Angeles is more than double the size of any previous CCS-5 study area.

In addition, he said, in August, the team delivered “two quick-turnaround analyses in only two days for DHS.” One was associated with the bombings in London. The other had to do with the imminent arrival of Hurricane Dennis. Since that time, he said, the Secretary of DHS himself has submitted an additional one-day turnaround request.

The program has significantly improved the “positive visibility” of Los Alamos National Laboratory, Smith said, “because of the sustained high-quality work in solving problems that nobody else in the world can solve.”

In recent weeks, positive articles and interview requests have poured in from news organizations including the Washington Post, the Discovery Channel, Time Magazine, CNN, NBC, CBS, Investor’s Business Daily, Wired News, and Men’s Health.

In addition, in the last six months, the team has produced 21 refereed publications that were either printed or accepted.

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Meet Our New People

Malcolm Andrews joined Los Alamos National Laboratory (LANL) on May 17 as the National Security Fellow and is working in Continuum Dynamics (CCS-2) and the Neutron Science and Technology Group (P-23).

His association with LANL stretches back some 18 years. He brings to the Laboratory hydro experience that involves the Rayleigh-Taylor and Richtmyer-Meshkov instabilities.

Originally from the United Kingdom, Andrews worked for a year (1976) at Winfrith (the United Kingdom Atomic Energy Authority), doing computational fluid dynamics.

He then earned bachelor’s and master’s degrees in mathematics from Oxford University.

After his studies at Oxford, he worked for three years at a computer scientific consultancy in London.

Subsequently, he earned a DIC (the equivalent of a master’s degree) and a Ph.D. in mechanical engineering from Imperial College in London. His doctoral thesis was on “Turbulent Mixing by Rayleigh-Taylor Instability.” His advisor was D. Brian Spalding, and his sponsor was David Youngs at Aldermaston, the English equivalent of LANL.

He came to the United States in 1986, working initially as a lecturer in the mechanical and aerospace engineering department at Princeton. He also did research in computational fluid dynamics of internal combustion engines and visited LANL as part of the DISC program in the Theoretical Division (T Division).

He then joined the faculty at Texas A&M in 1991, becoming a full professor in 2004.

Both he and his wife, Farzaneh F. Jebrail, became U.S. citizens in 1997.

Malcolm has chosen a house on 48th Street in Los Alamos and is settling in well. His wife, who holds a Ph.D. in chemical engineering (with expertise in experimental combustion and heat transfer) is working in the Advanced Chemical Diagnostics and Instrumentation Group (C-ADI) and is a program manager for buildings and industrial technology in the Office of Energy and Environment Initiatives (OEEI).

(Please see **ANDREWS** on Page 5.)

ANDREWS (Cont'd from p.4.)

His daughter Nasim, 10, is now a student at Mountain Elementary School, and, he said, "She loves it."

Andrews is no stranger to LANL. "I've worked with Lab scientists for 18 years," he said, mentioning Frank Harlow, Peter O'Rourke, Guy DiMonte, Robert Benjamin, and Kathy Prestridge.

His work at LANL involves theory, computation, and experiments, primarily associated with hydro mix, with applications to inertial confinement fusion, engines, aerosols, and turbulence.

Graham Mark, who joined the Discrete Simulation Science Group (CCS-5) recently, is the son of J. Carson Mark, noted Manhattan Project mathematician/physicist, who came to Los Alamos in 1945 and subsequently led the Theoretical Division for 26 years.

Graham was born in Canada. He moved with his family to Los Alamos in 1945, when he was six weeks old. He grew up in Los Alamos and graduated from Los Alamos High School. After earning a bachelor's degree in mathematics from the University of Colorado, he worked at the Laboratory for a year in the Meson Physics Division (MP), helping in early designs of the Los Alamos Meson Physics Facility (LAMPF) and learning the FORTRAN programming language.

He attended the University of New Mexico (UNM), working on a master's degree in United States history. He also attended UNM Law School for a year. He eventually discovered biology and obtained a master's degree in plant ecology from UNM. He earned his doctorate in evolutionary biology from the State University of New York at Stony Brook and proceeded to a three-year postdoctoral position at Cornell University. Research for his Ph.D. concerned laboratory studies of a tiny beetle's evolutionary responses to heterogeneous environments. His postdoctoral work consisted of laboratory studies of co-evolution of a host (housefly) and parasite (parasitic wasp). During this work, he increasingly used computers for statistical analyses.

Evolutionary biology, he found, offers few jobs outside of molecular work. On completing his postdoctoral work, with no jobs in sight and two small children, Graham accepted a job as a programmer at the Laboratory. He has worked at Los Alamos in that field ever since, through numerous reorganizations and renamings of the computer divisions.

About 10 years ago he joined the Scientific Software Engineering Group (CCN-12). That group provides programmers for hire throughout the Laboratory, and group members have opportunities in a wide variety of projects. Graham's work included a graphical user interface for a miniaturized flow cytometer (for which he obtained a patent), the Parallel Object-Oriented Methods and Applications scientific library, bioinformatics in the Human Genome Project,

graphical displays of results of DNA microarrays, and software to detect DNA "signatures." He worked briefly on TRANSIMS and got to know some of the people in the group that is now called CCS-5.

Graham was "hired" by CCS-5 in the spring of 2004. He found its work fascinating, innovative, and useful; its people interesting, varied, and friendly. He formally left CCN-12 and joined CCS-5 last spring.

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Security Tip

If you have not yet acquired a personal identification number (PIN) for Technical Area 3, it is essential that you do so soon.

This fall/winter, several TA-3 gates will go to a mechanized security system that requires a PIN as well as a badge swipe and palm reader for entry. One of the gates affected will be the "Chicken Shack."

Laboratory employees who didn't obtain a PIN during the regular sign-up period may go to the Badge Office during the week of October 11-14.

The process is relatively simple: Swipe your badge, enter a PIN of at least four digits, and then place your palm in the reader. Once the number has been confirmed, you're done.

Just don't forget the number.

In Case You Missed It....

The Los Alamos Computer Science Institute (LACSI) will be held October 11 through 13 in Santa Fe. For full information on all 10 full-day sessions at LACSI, see <http://lacsi.rice.edu/symposium> and click on "LACSI Workshop Program." Seven of the 10 are co-produced by Los Alamos National Laboratory scientists, many of them from CCS.

SC05 Gateway to Discovery is scheduled November 12 through 18 at the Washington State Convention and Trade Center in Seattle. Bill Gates will deliver the keynote address this year. For further details on the conference, go to <http://sc05.supercomputing.org/home.html>.

The Computer and Computational Sciences Division will have a booth at this year's conference. **Becky Fernandez**, CCS-Division Office, 665-4700, is the contact for the booth.

Wu Feng, CCS-1, will serve as the moderator for two of the four panels featured at SC05—the panel entitled "Tour de HPCycles," and the panel on "The Six-Million Processor System."

Cindy Sievers, CCS-1, will be the general producer of the SC Global Showcase at the conference: http://sc05.supercomputing.org/programs/sc_global.php.

(Please see IN CASE on page 6.)

IN CASE (Cont'd from p.5.)

Sievers noted that SC Global will have audiences not only in Seattle but all over the world during the conference. For full details on the SC Global

Showcase, go to:

http://sc05.supercomputing.org/programs/sc_global_showcase.php.

One new feature at the conference this year will be SC Desktop, which will allow participants to pay a reduced registration fee, download the necessary software, and view many portions of the SC05 program from their desktops. For more information on this feature, access:

http://sc05.supercomputing.org/programs/sc_global_desktop.php.

Don Hush and James Howse, both of CCS-3, were the hosts for a recent workshop on "Machine Learning for Semantic Networks" as part of the ADVISE project for the Department of Homeland Security. They presented a talk on "Anomaly Detection on Graphs." The workshop had invited speakers including Tina Eliassi-Rad from Lawrence Livermore National Laboratory, Phillip Kegelmeyer from Sandia National Laboratories-California, Tom Potok from Oak Ridge National Laboratory, and Christian Posse from Pacific Northwest National Laboratory. Among those who attended were **Cliff Joslyn, Karin Verspoor, Susan Mniszewski, Levi Larkey, and Reid Riverburgh**, all from CCS-3.

Daryl Holm of CCS-2 recently gave a plenary talk at the United Kingdom Royal Meteorological Society biennial meeting at Exeter University. His talk, "Lagrangian Averaged Equations for Modelling Turbulent Circulations," drew on "crucial input" supplied by **Matthew Hecht and Mark Petersen**, both of CCS-2. The talk summarized the development and tests of the Lagrangian averaged Navier Stokes alpha equations at Los Alamos over the past seven years. It discussed the application of the alpha equations in geophysical flows, particularly in ocean circulation modeling. In one of the highlights of his presentation, Holm reported on the alpha model's preservation of variability at coarse resolution in geophysical flows found recently in his joint work with **Balu Nadiga** and **Beth Wingate**, also of CCS-2.

David Carrington, CCS-4, (in collaboration with Darrell Pepper from the University of Nevada), is the author of a chapter on indoor air pollution modeling in the recently published book *Air Quality Modeling, Theories, Methodologies, Computational Techniques, and Available Databases and Software, Volume II—*

Advanced Topics. To see a flyer on the gook, go to http://envirocomp.org/aqm/AQM2_flyer.pdf.

CCS Division Leader William J. Feiereisen, chairman of the Division Leaders Council, will serve on the Laboratory Hiring Council announced September 28 by Laboratory Director Robert W. Kuckuck. Because of tight budget projections for the next two years, this committee will review all new postings and hiring requests at the Laboratory.

Beth Wingate, CCS-2, was selected by the Women's Diversity Working Group to receive one of the 10 Women's Career Development Mentoring Awards this year.

The award recognizes persons who provide exemplary mentoring supporting the career development of women at the Laboratory.

Mark Christon of CCS-2 is taking a personal leave of absence to deal with family issues. CCS Deputy Division Leader Stephen Lee said (in his most recent weekly update), "We're glad to have gotten to know him, are thankful for his contributions to a number of projects, and wish him all the best."

The 4th Annual CCN-CCS Golf Tournament will be held on Friday, October 7. All CCN and CCS personnel are invited to participate.

A note from **Ray Miller** said, "This year we will be doing a shotgun start on Friday, October 7, for up to 12 foursomes at the Los Alamos Golf Course on Diamond Drive in Los Alamos. The start time is 9 a.m. There will be a cookout afterwards on the patio at the golf course. Soft drinks will be provided.... This is intended to be social outing as much as a golf tournament. All abilities are welcome. This year we need volunteers (two to three people) to help with cooking of the food in order to accomplish the tournament."

For full details on the foursomes, the fees, etc., contact Miller at rdm@lanl.gov.

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Editor's Note

Our apologies for the lack of illustrations in this issue. As we were preparing stories for the newsletter, it became obvious that the CCS News Bytes printer was malfunctioning. All of the photos we printed had strong vertical stripes. We assumed that we would not be able to print photos acceptably, and, as a result, prepared none. The problem is fixed now. We hope the next issue can feature pictures again.

Charmian Schaller